Vacuum polarization by a strong coulomb field and its contribution to the spectra of multiply-charged ions

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Vacuum polarization by a point charge Z is calculated rigorously without using an expansion in the parameter αZ. The corresponding correction to the energy levels of hydrogen-like ions with Z between 10 and 137 is calculated, and substantially reduces the uncertainty in theoretical estimates of the level energies of multiply charged ions. An asymptotic expansion is obtained analytically for the polarization potential at large distances from the nucleus.

1. INTRODUCTION

Although quantum electrodynamics has been successful in describing the interaction between free electrons and photons, the computational difficulties encountered in the case of bound states are so much greater that even calculations of lowest-order radiative corrections in α have to be considered separately in each special case, and require the use of powerful computers. Thus, the energy shift in hydrogen-like ions was calculated in the late 1940s to lowest order in αZ (Z is the nuclear charge), but the precise calculation that did not involve an expansion in αZ was not carried out until 1975 (Refs. 1 and 2), and is the only example of an exact evaluation of the quantum electrodynamic corrections to the energy levels of high-Z atoms. In the present paper, we report an analogous evaluation of another diagram in the lowest order in α that contributes to the Lamb shift, namely, the vacuum polarization effect. In view of experimental advances (e.g., in the spectroscopy of mesic atoms and of multiply-charged ions, and in collisions between heavy nuclei), accurate calculations of the polarization of vacuum by a high-Z Coulomb center is of both theoretical and practical interest. In particular, the main uncertainty in theoretical estimates of the energy levels of heavy ions[3] is currently due to a lack of accurate calculations of the vacuum polarization diagram.

Vacuum polarization produces a "smearing out" of the point charge eZ, so that the charge density distribution assumes the form[4]

$$\rho(r)=eZ\delta(\mathbf{r})+\rho^{(1)}(r)+\rho^{(3)}(r)+\rho^{(5)}(r)+\dots$$
$$=eZ\delta(\mathbf{r})+\rho^{(1)}+\rho^{(3+)}(r),\quad e\rho^{(n)}(r)\sim\alpha(\alpha Z)^n$$

where r is the distance from the nucleus. We shall write the potential due to this charge distribution in the form

$$V(r)=eZ/r+V^{(1)}(r)+V^{(3+)}(r),$$

where $V^{(1)}$ is the well known Uehling potential which is linear in Z (Ref. 5) and $V^{(3+)}$ contains terms that are nonlinear in Z. The question of vacuum polarization by a strong Coulomb field was first examined in Ref. 4 in which general expressions were obtained for $V^{(3+)}$ and for the point charge Q that appears in $\rho^{(3+)}$ and determines $V^{(3+)}$ for small r:

$$V^{(3+)}\approx Q/r,\quad r\to 0.$$

However, the expressions for $V^{(3+)}$ are found to be very complicated. They were simplified to some extent in a later paper,[6] but only for the part of the potential that was cubic in Z, and the expression $V^{(3)}$ was used in various calculations (see for example Ref. 3).

Vacuum polarization was subsequently investigated analytically and numerically by several workers, but the results obtained were valid mostly for small distances $r\lesssim\lambda_e$ ($\lambda_e=\hbar/mc$), which are significant in mesic atoms and superheavy ions with $\alpha Z>1$. The first few terms in the expansion of $V^{(3+)}$ for small r were obtained in Refs. 7 and 8. In particular, a simple expression was found for the point charge Q (see also Ref. 9). In Refs. 10 and 11, a numerical calculation of $\rho^{(3+)}$ was made, using the Coulomb Green's function and taking into account only the first term in the partial expansion [*cf.* the term with $k=1$ in (2)]. In Ref. 12, $\rho^{(3+)}$ was calculated by direct summation over the state of the electron and positron in the Coulomb potential, taking into account a few terms of the partial expansion. It was then used in Refs. 10–12 to calculate the energy level shifts in mesic atoms and heavy ions, so that the finite size of the nucleus had to be taken into account.

In the present paper, we report a complete calculation of $V^{(3+)}$ for a point nucleus with $Z\leqslant 137$. The overall scheme of the calculation (Sec. 2) is closest to that used in Ref. 10. Asymptotic expansions are obtained for $V^{(3+)}$ and for the partial terms $\rho_k(r)$ (Sec. 3) for large r. These enable us to develop a technique for calculating $V^{(3+)}$ for all r (Sec. 4). The results obtained in this way are used to calculate the energy level shifts for the states $|nlj\rangle$ of hydrogen-like ions with $n=1-5$, $l=0-2$ (Sec. 5).

2. GENERAL FORMULAS

The expression for the density of induced charge in terms of the exact Feynman propagator $S_F(x,x')$ for the motion of an electron in the Coulomb field of the nucleus is given by the well-known expression[10]

$$\rho=ie\,\mathrm{Sp}(S_F(x,x')\gamma_0)|_{x'\to x},$$

where the matrices γ are chosen in the standard manner and the charge of the electron $-e$. If we write S_F as a Fourier integral of the Coulomb Green's function $G(\mathbf{r},\mathbf{r}',E)$, and rotate the contour of integration on the complex plane of E around the imaginary axis, we obtain

$$\eta=-\frac{e}{2\pi}\int_{-\infty}^{\infty}d\omega\,\mathrm{Sp}\,G(\mathbf{r},\mathbf{r}';i\omega)\gamma_0|_{\mathbf{r}'\to\mathbf{r}}. \qquad (1)$$

If we then use the following partial expansion for G:

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$$G(\mathbf{r},\mathbf{r}';E)=\sum_{JLM}\begin{vmatrix} G^{(1)}_{JL}(r,r';E)\,Y_{LL}(\mathbf{n},\mathbf{n}'), & iG^{(2)}_{JL}(r,r';E)\,Y_{LL'}(\mathbf{n},\mathbf{n}') \\ iG^{(3)}_{JL}(r,r';E)\,Y_{L'L}(\mathbf{n},\mathbf{n}'), & -G^{(4)}_{JL}(r,r',E)\,Y_{L'L'}(\mathbf{n},\mathbf{n}') \end{vmatrix},$$

where $\mathbf{Y}_{L_1L_2}(\mathbf{n},\mathbf{n}')=\Omega_{JL_1M}(\mathbf{n})\Omega_{JL_2M}(\mathbf{n}')$, Ω_{JLM} is the spherical bispinor, and $L'=2J-L$, we obtain the following expression after summation over M and evaluation of the trace in (1):

$$\rho(r)=\sum_{k=1}^{\infty}k\rho_k(r),\quad k=J+{}^1/_2, \tag{2}$$

where

$$\rho_{J+1/2}(r)=-\frac{e}{4\pi^2}\sum_{L=J\pm1/2}\int_{-\infty}^{\infty}d\omega\,[G^{(1)}_{JL}(r,r;i\omega)+G^{(4)}_{JL}(r,r;i\omega)]. \tag{3}$$

We have put $r'=r$ in the above expressions because the partial terms $G^{(\alpha)}_{JL}(r,r';E)$ are finite for $r'\to r$. Using the expression for G_{JL} in terms of the Whittaker functions $M_{\eta,\gamma}$ and $W_{\eta,\gamma}$ (see, for example, Ref. 13), we obtain

$$\rho_k(r)=-\frac{e}{4\pi^2r^3}\int_0^{\infty}g_k(\omega,r)\,d\omega, \tag{4}$$

where

$$g_k(\omega,r)=-\mathrm{Re}\,\frac{2\Gamma(\gamma-\eta)}{(1+\omega^2)\Gamma(2\gamma+1)}\{Z\nu[(\gamma-\eta)M_-W_-+M_+W_+] +i\omega(\gamma-\eta)[M_-W_+-(\gamma+\eta)M_+W_-]\}, \tag{5}$$

$$\gamma=(k^2-(\alpha Z^2))^{1/2},\quad \nu=\alpha/(1+\omega^2)^{1/2},\quad \eta=i\omega Z\nu,\quad x=2r(1+\omega^2)^{1/2},$$

$\Gamma(x)$ is the gamma function, and $M_{\pm}=M_{\eta\pm1/2,\gamma}(x)$, $W_{\pm}=W_{\eta\pm1/2,\gamma}(x)$. We have changed the limits of integration with respect to ω between (3) and (4) in view of the symmetry of the integrand.

The above expressions for ρ do not converge. The divergence in (1) is due to the singularity $G(\mathbf{r},\mathbf{r}';E)\sim|\mathbf{r}'-\mathbf{r}|^{-1}$ for $\mathbf{r}'\to\mathbf{r}$. The quantity $\rho_k(r)$ is finite in (3) and (4), but the sum over λ in (2) does not converge. The expression for ρ is conveniently regularized by subtracting from (4) the part of $\rho_k(r)$ that is linear in Z (Refs. 10–12). This removes from $\rho_k(r)$ the part of the induced charge density that corresponds to the Uehling potential, which is very convenient in the evaluation of $\rho^{(3+)}$. After this subtraction, the expression for $\rho^{(3+)}$ is found to be finite, but contains ambiguities because the diagram for $\rho^{(3)}$ with four vertices has to be renormalized. This ambiguity is reflected in the fact that the values of $\rho^{(3+)}$ are found to be different if we alter the order of summation over the k and integration with respect to ω in (2) and (4). It is shown in Refs. 10 and 12 that the additional renormalization is unnecessary when integration with respect to ω is carried out in each partial term ρ_k in (4), followed by summation over k in (2).

Thus, the renormalized expression for ρ_k is

$$\rho_k^{(3+)}(r)=-\frac{e}{4\pi^2r^3}\int_0^{\infty}(g_k(\omega,r)-g_k^{lin}(\omega,r))\,d\omega, \tag{6}$$

where the part that is linear in Z, i.e.,

$$g_k^{lin}(\omega,r)=Z\left[\frac{\partial}{\partial Z}g_k(\omega,r)\right]\Big|_{Z=0}$$

can be written in the form

$$g_k^{lin}(\omega,r)=-\frac{2\alpha Z(k-1)!}{(1+\omega^2)^{k/2}(2k)!}\{kM_-W_-+M_+W_+ +\omega^2[(1+k\psi(k))M_-W_+ -k(M_-'W_+ +M_-W_+')+k^2(M_+'W_- +M_+W_-'-\psi(k)M_+W_-)]\}$$

in which

$$\psi(x)=\frac{d}{dx}\ln\Gamma(x),\quad M_{\pm}=M_{\pm1/2,k}(x),$$
$$W_{\pm}=W_{\pm1/2,k}(x),\quad M_{\pm}'=\frac{d}{d\eta}M_{\eta\pm1/2,k}(x)\,|_{\eta=0},$$
$$W_{\pm}'=\frac{d}{d\eta}W_{\eta\pm1/2,k}(x)\,|_{\eta=0}. \tag{7}$$

The explicit expressions for the derivatives $M'_{\pm}$ and $W'_{\pm}$ are given in the Appendix.

3. ASYMPTOTIC EXPRESSIONS FOR ρ AND V

An analytic examination of $\rho^{(3+)}(r)$ is possible only for small and large r. The expansions for $r\to0$ are discussed in the Introduction, so that we shall confine our attention to the case $r\gg\lambda_c$. To determine $\rho^{(3+)}$, we must find the asymptotic behavior of $\rho_k^{(3+)}(r)$ for large r and k. To obtain the necessary expansions for the integral (6), it is convenient to write $g_k(\omega,r)$ in (5) in the form

$$g_k(\omega,r)=-\mathrm{Re}\,\frac{1}{1+\omega^2}\left\{Z\nu(T_++T_-) +i\omega\left[(x-\eta-1)T_++x\frac{d}{dx}T_+\right]\right\}, \tag{8}$$

where

$$T_{\pm}=T(\eta\pm{}^1/_2,\gamma,x),$$

$$T(\eta,\gamma,x)=\frac{\Gamma(\gamma-\eta+{}^1/_2)}{\Gamma(2\gamma+1)}M_{\eta,\gamma}(x)\,W_{\eta,\gamma}(x).$$

As in the general case of a product of any two solutions of a linear second order differential equation, we can write the following third-order equation for $T(\eta,\gamma,x)$:

$$x^2\frac{d^3T}{dx^3}-[x^2-4\eta x+4\gamma^2-1]\frac{dT}{dx}-\left(2\eta-\frac{4\gamma^2-1}{x}\right)T=0, \tag{9}$$

which is convenient for obtaining the asymptotic expansion for $T_{\pm}$.

Since γ is finite for $x\to\infty$ (this corresponds to large r and finite k), T can be written in the form

$$T(\eta,\gamma,x)=\sum_{n=0}^{\infty}a_n x^{-n}, \tag{10}$$

where $a_0=1$, which follows from the known asymptotic behavior of M and W (Ref. 14), and a_n for $n>0$ is found from the recurrence relation

$$(n+1)a_{n+1}=2\eta(2n+1)a_n+n(n^2-4\gamma^2)a_{n-1}, \tag{11}$$

which follows from (9). The solution of (11) is

$$a_n=\sum_{m=0}^{n}\sum_{l=0}^{[(n-m)/2]}a_{mnl}(-\gamma^2)^l\left(\eta-\frac{1}{2}\right)^m, \tag{12}$$

where a_{mnl} are positive integers. The expansions given by (10) and (12) enable us to write $g_k(\omega,r)$ in the form of a series, where the integral (6) with respect to ω can be evaluated analytically:

$$\frac{4\pi^2}{e}\rho_k^{(3+)}(r)=\sum_{m=0}^{\infty}r^{-2m-9}\sum_{n=1}^{[(m+2)/2]}\sum_{l=0}^{m-2n+2}h_{mnl}(\alpha Z)^{2n+1}k^{2l}$$

$$=(\alpha Z)^3r^{-9}\left\{\frac{16}{15}+\left(\frac{640}{21}-\frac{64}{15}k^2\right)r^{-2}\right.$$

$$+\left[\frac{61\,920}{63}-\frac{5200}{21}k^2+\frac{16}{15}k^4\right.$$

$$\left.\left.+\frac{64}{21}(\alpha Z)^2\right]r^{-4}+\ldots\right\} \tag{13}$$

Henceforth we use relativistic units for which $\hbar=m=c=1$.

For large $k\sim r$ ($\gamma\sim x$), we can find the asymptotic behavior of T by substituting $x=by$, $b=(4\gamma^2-1)^{1/2}$ in (9) and take T in the form

$$T(\eta,\gamma,x)=\sum_{n=0}^{\infty}T^{(n)}(y)\,b^{-n}. \tag{14}$$

A set of coupled differential equations is thus obtained for $T^{(n)}$ from (9). Its solution is

$$T^{(n)}(y)=\sum_{l=1}^{m+1}\sum_{m=1}^{3n+1}C_{nlm}\frac{\eta^{l-1}y^l}{(1+y^2)^{m-1/2}}, \tag{15}$$

where C_{nlm} are rotational numbers ($C_{011}=1$) that can be determined recursively.

Evaluating the integral with respect to ω in (6), and using (14) and (15), we obtain the following expression for $\rho_k^{(3+)}(r)$:

$$\rho_k^{(3+)}(r)=\frac{e}{4\pi^2}\sum_{m=1}^{\infty}d_m r^{-2m-7}, \tag{16}$$

$$d_m=\sum_{n=1}^{[(m+1)/2]}\sum_{l=1}^{2m-2n+1}e_{nlm}(\alpha Z)^{2l+1}p(r)^{n+m+2} \tag{17}$$

where e_{nlm} are rational numbers that can be expressed in terms of C_{nlm}, $p(r)=r^2(r^2+k^2-1/4)^{-1}$. The first few terms of the expansion for $\rho_k^{(3+)}(r)$ are

$$\rho_k^{(3+)}(r)=\frac{e(\alpha Z)^3}{4\pi^2}p^4r^{-9}\left\{\frac{16}{15}-\left(\frac{64}{35}+\frac{688}{21}p-64p^2\right)\frac{p}{r^2}\right.$$

$$+\left[\frac{142}{35}-\frac{5464}{105}p+\frac{37\,072}{15}p^2-\frac{130\,048}{15}p^3\right.$$

$$\left.\left.+7168p^4+\frac{64}{21}(\alpha Z)^2\right]\frac{p^2}{r^4}+\ldots\right\}. \tag{18}$$

Substituting (16) and (17) in (2) and summing over k term by term with the aid of the well-known Euler–Maclaurin formula [it is convenient to use the expansion (13) for $\rho_k^{(3+)}$ to calculate the derivatives in these expressions], we finally obtain

$$\rho^{(3+)}(r)=\frac{e}{4\pi^2}\sum_{m=0}^{\infty}\sum_{n=1}^{[(m+2)/2]}(m!)^2(2m+4)$$

$$\times(2m+5)f_{mn}\frac{(\alpha Z)^{2n+1}}{r^{2m+7}}. \tag{19}$$

We also supply an analytic expression for the potential $V^{(3+)}(r)$. Since the induced charge must be zero, i.e.,

$$\int_0^{\infty}r^2\rho^{(3+)}(r)\,dr=0, \tag{20}$$

we have

$$V^{(3+)}(r)=-4\pi\int_r^{\infty}r'\left(\frac{r'}{r}-1\right)\rho^{(3+)}(r')\,dr'. \tag{21}$$

Substituting (19) in (21), we obtain the following expression for the energy of an electron in the potential $V^{(3+)}$:

$$U^{(3+)}(r)=-eV^{(3+)}(r)$$

$$=\frac{\alpha}{\pi}\sum_{m=0}^{\infty}\sum_{n=1}^{[(m+2)/2]}(m!)^2f_{mn}(\alpha Z)^{2n+1}r^{-2m-5}. \tag{22}$$

The first few terms of this expansion are

$$U^{(3+)}(r)=\frac{\alpha(\alpha Z)^3}{\pi}\left[\frac{2}{225r^5}+\frac{59}{1323r^7}+\frac{1977+20(\alpha Z)^2}{4725r^9}\right.$$

$$+\frac{12\,5860+34\,144(\alpha Z)^2}{190\,575r^{11}}$$

$$\left.+\frac{1\,960\,420\,032+93\,618\,070(\alpha Z)^2+96\,096(\alpha Z)^4}{12\,297\,285r^{13}}+\ldots\right].$$

Table I lists the higher-order coefficients f_{mn} for $m=5$–12, $n=1$–4. We note that earlier papers reproduce only the first term of the asymptotic form of $U_r^{(3+)}$ (Ref. 14; see also Ref.

TABLE I. Values of the coefficients f_{mn}.

m	n			
	1	2	3	4
5	0,3812769	0,0266795	0,0000860	0
6	0,4946161	0,0458093	0,0002918	$6\cdot10^{-8}$
7	0,6150374	0,0707397	0,0007216	$5\cdot10^{-7}$
8	0,7412290	0,1014082	0,0014705	$23\cdot10^{-7}$
9	0,8721898	0,1376368	0,0026288	$69\cdot10^{-7}$
10	1,0071432	0,1791838	0,0042776	$167\cdot10^{-7}$
11	1,1454776	0,2257770	0,0064866	$346\cdot10^{-7}$
12	1,2867042	0,2771342	0,0093134	$643\cdot10^{-7}$

15), which can be interpreted in terms of the Lagrangian for the uniform electromagnetic field.

4. NUMERICAL DETERMINATION OF CHARGE DENSITY AND POTENTIAL

The functions $\rho^{(3+)}(r)$ and $V^{(3+)}(r)$ were calculated accurately using (2)–(7) and (21). The function $M_{\eta,\gamma}(x)$ was calculated either by expanding it into a series or by using the asymptotic expansion in terms of x. The function $W_{\eta,\gamma}(x)$ has a range of intermediate values of x in which both these expressions yield values of low precision. It is then more effective to use the ε-algorithm[16] for the asymptotic expansion for W. There is some loss of precision for small Z when the difference $g_k - g_k^{lin}$ in (6) is evaluated because $(g_k - g_k^{lin})/g_k \sim (\alpha Z)^2$. The calculations were therefore performed only for $Z \geqslant 10$.

The integral with respect to ω in (4) was evaluated numerically, using Gauss quadratures between 0 and ω_0, and analytically between ω_0 and ∞, using the asymptotic expansion for $g_k(\omega,r)$, obtained from (10). It is important to note that the integrand in (6) is a smooth function of ω that changes sign only once on the interval $(0,\infty)$, but the total integral with respect to ω is found to be 3–7 orders of magnitude smaller (as a function of r) than the integral of $|g_k - g_k^{lin}|$, and this means that the final answer is accurate to a smaller number of significant figures.

This evaluation of $\rho_k^{(3+)}(r)$ was performed only for $k = 1$–7. For $k \geqslant 8$, the function $\rho_k^{(3+)}(r)$ was calculated using the asymptotic expansion (16). For $r \sim k \sim 15$, up to twelve expansion terms had to be included to achieve a relative precision of 10^{-7}. For $r > 15$, the required precision is obtained with (19) for $\rho^{(3+)}(r)$. The summation over k in (2) presents no difficulty. For small r, the terms in the sum over k fall rapidly, whereas for large r the main contribution is provided by the region $k \simeq r$ [it follows from (16) that the expression for $k\rho_k^{(3+)}(r)$ has a maximum at $k \approx r/\sqrt{15}$]. Figure 1 shows the relative contribution of $k\rho_k^{(3+)}(r)$ to $\rho^{(3+)}(r)$ for $k = 1$–4 and $Z = 82$.

The above procedure was used to calculate the functions $\rho^{(3+)}(r)$, $V^{(3+)}(r)$ throughout the interval $0 < r < \infty$ and $Z \leqslant 137$ with relative precision of 10^{-6} or better. The value $\alpha^{-1} = 137.036$ was used in the numerical calculations. An additional check on the precision was made by verifying that the total induced charge was

$$\int_\varepsilon^\infty r^2\rho^{(3+)}(r)\,dr + Q = 0, \quad \varepsilon \to +0,$$

where Q is the induced point charge calculated from the analytic formulas.[7–9] Figure 2 shows the r dependence of the function

$$f(r, Z) = rU^{(3+)}(r)/\alpha(\alpha Z)^3$$

for several values of Z. We note that the $f(r, Z = 0)$ curve corresponds to the potential $V^{(3)}$, calculated from the formulas given in Ref. 6, and that $f(r = 0, Z) = Q/\alpha(\alpha Z)^3$.

5. CONTRIBUTION OF VACUUM POLARIZATION TO THE ENERGY-LEVEL SHIFT IN HYDROGEN-LIKE IONS

The energy shift is calculated in the usual way:

$$\Delta E_{nlj} = \langle nlj | U^{(1)} + U^{(3+)} | nlj \rangle = \Delta E_{nlj}^{(1)} + \Delta E_{nlj}^{(3+)}, \qquad (23)$$

where we have taken into account the contribution of the

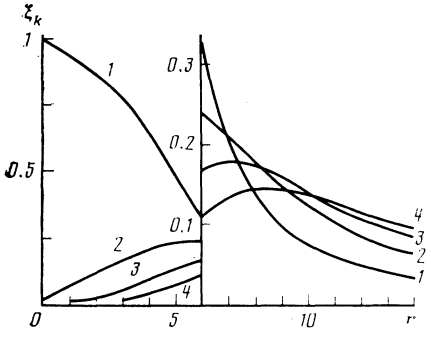

FIG. 1. The ratio $\xi_k = k\rho_k^{(3+)}/\rho^{(3+)}$ as a function of r for $Z = 82$. The traces are labeled with the values of k.

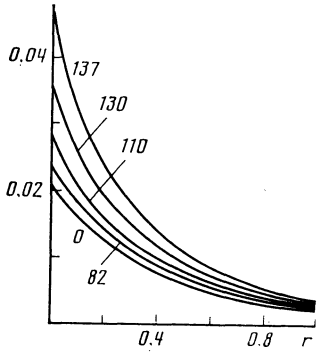

FIG. 2. The radial function $f(r,Z) = rU^{(3+)}/\alpha(\alpha Z)^3$. The traces are labeled with the values of Z.

Uehling potential $\Delta E^{(1)}$ and of the terms nonlinear in Z. We begin with the case $\alpha Z \ll 1$. The matrix elements of $U^{(1)}$ can then be evaluated by replacing the bispinor $\Psi_{nlj}(r)$ with its expansion for $r \to 0$. In the lowest order in αZ, we have

$$\Delta E^{(1)}_{nlj}(\alpha Z \to 0) = -\alpha \left(\frac{2\alpha Z}{n}\right)^{2l+4} \frac{(n+l)!\,(l!)^2}{8\pi(2l+3)[(2l+1)!]^2(n-l-1)!} \times \left[\frac{l+2}{2l+5} + \frac{(2l+1)(l+1)}{4l^2}\delta_{l,j+1/2}\right]. \quad (24)$$

We note that the expression for $\Delta E^{(1)}_{nlj}(\alpha Z \to 0)$ given in Ref. 13 (Page 77) does not include the term containing $\delta_{l,j+1/2}$, due to a small component of Ψ_{nlj}. It follows that, when the contribution of the Uehling potential is estimated, we cannot use the nonrelativistic hydrogen wave functions even to lowest order in αZ. For small Z, the quantity $\Delta E^{(3+)}_{nlj}$ is determined exclusively by the term $V^{(3)}$ in the potential $V^{(3+)}$, and can be obtained by recalling that, for small Z, the Bohr radius a_0 is significantly greater than the characteristic length for a change in $V^{(3)}(r)$. For $l=0$, the quantity $\Delta E^{(3+)}_{nlj}$ $(\alpha Z \to 0)$ is determined by the behavior of the wave function for $r \sim 1 \ll a_0$, whereas for $l \geqslant 2$, it is determined by the region $r \simeq a_0 \gg 1$ in which we can use the asymptotic form of $V^{(3+)}$. For $l=1$, we must take into account the contribution of both regions ($r \simeq 1$ and $r \simeq a_0$). The expression for $\Delta E^{(3+)}_{nlj}$ for $\alpha Z \to 0$ is

$$\Delta E^{(3+)}_{nlj}(\alpha Z \to 0) = \begin{cases} \dfrac{4\alpha(\alpha Z)^6}{n^3} b_2, & l=0, \\ \dfrac{4\alpha(\alpha Z)^8(n^2-1)}{9n^5}\left[\dfrac{2}{225\pi}\left(-\ln\dfrac{2\alpha Z}{n} + C_n - C\right) + b_4 + \dfrac{9}{4}b_2\delta_{1,j+1/2}\right], & l=1, \\ \dfrac{128\alpha(\alpha Z)^8(5n^2-3l^2-3l+1)(2l-3)!}{225\pi n^5(2l+4)!}, & l \geqslant 2. \end{cases} \quad (25)$$

where

$$b_2 = \frac{1}{\alpha(\alpha Z)^3}\int_0^\infty r^2 U^{(3)}(r)\,dr = 0{,}0045105564,$$

$$b_4 = \frac{1}{\alpha(\alpha Z)^3}\left[\int_0^1 r^4 U^{(3)}(r)\,dr + \int_1^\infty \left(r^4 U^{(3)}(r) - \frac{2\alpha(\alpha Z)^3}{225\pi r}\right)dr\right]$$

$$= 0{,}004252588$$

$$C_n = \int_0^\infty (r^{-5} M^2_{n,1/2}(r) - r^{-4}e^{-r})\,dr,$$

$C_2 = 0$, $C_3 = -7/16$, $C_4 = -147/200$, $C_5 = -77/80$, and $C = 0.57721566...$ is the Euler constant. The results of numerical calculations are conveniently written in the form

$$\Delta E^{(3+)}_{nlj} = \left(1 + \frac{\delta_{j,1/2}}{[1-(\alpha Z)^2]^{1/2}}\right) F_{nlj}(\alpha Z)\,\Delta E^{(3+)}_{nlj}(\alpha Z \to 0), \quad (26)$$

where F is a smooth function of Z. Table II lists the values of F for states with $n = 1$–5, $l = 0,1,2$.

The calculated energy levels of hydrogen-like ions with allowance for radiative corrections, and also for recoil and nuclear structure effects, are gathered together in Ref. 3, where the potential $V^{(3)}$ was used to estimate $\Delta E^{(3+)}$. Comparison with our results shows that the use of $V^{(3)}$ instead of $V^{(3+)}$ leads to a result that is too low. Thus, for $Z = 82$, the

TABLE II. Values of the function $F_{nlj}(\alpha Z)$.

nlj	Z						
	10	20	82	100	110	130	137
$1s_{1/2}$	0,4328	0,3896	0,3479	0,4073	0,4749	0,9135	2,4351
$2s_{1/2}$	0,4336	0,3931	0,4315	0,5788	0,7464	1,9541	6,7830
$3s_{1/2}$	0,4335	0,3929	0,4285	0,5709	0,7310	1,8360	5,8460
$4s_{1/2}$	0,4334	0,3925	0,4205	0,5528	0,6997	1,6737	4,9360
$5s_{1/2}$	0,4333	0,3921	0,4139	0,5382	0,6751	1,5585	4,3697
$2p_{1/2}$	0,4825	0,4786	0,8359	1,2782	1,7866	5,9115	27,862
$3p_{1/2}$	0,4822	0,4779	0,8149	1,2205	1,6745	5,0967	20,575
$4p_{1/2}$	0,4820	0,4772	0,7936	1,1663	1,5750	4,5016	16,536
$5p_{1/2}$	0,4819	0,4768	0,7779	1,1279	1,5064	4,1289	14,319
$2p_{3/2}$	0,9550	0,9166	0,9081	0,9936	1,0708	1,3589	1,6509
$3p_{3/2}$	0,9554	0,9187	0,9574	1,0778	1,1835	1,5717	1,9485
$4p_{3/2}$	0,9555	0,9191	0,9682	1,0966	1,2091	1,6218	2,0197
$5p_{3/2}$	0,9554	0,9191	0,9699	1,0996	1,2133	1,6302	2,0321
$3d_{3/2}$	1,0942	1,3001	4,2302	5,9125	7,1949	11,319	14,594
$4d_{3/2}$	1,1052	1,3355	4,6060	6,4957	7,9411	12,611	16,342
$5d_{3/2}$	1,1096	1,3493	4,7415	6,6965	8,1904	13,014	16,874
$3d_{5/2}$	1,0341	1,1020	1,7385	1,9898	2,1592	2,6502	3,0625
$4d_{5/2}$	1,0385	1,1152	1,8570	2,1622	2,3707	2,9804	3,4865
$5d_{5/2}$	1,0402	1,1205	1,9037	2,2301	2,4542	3,1119	3,6564

TABLE III. Values of the corrections $\Delta E^{(1)}$, $\Delta E^{(3)}$, and $\Delta E^{(3+)}$, $\Delta E^{(s)} = \frac{\alpha(\alpha Z)^4}{\pi} F^{(s)} mc^2$.

	Z			
	55	82	92	100
$F^{(1)}$	−0,2584	−0,3409	−0,4064	−0,4890
$F^{(3)}$	0,0060	0,0142	0,0194	0,0252
$F^{(3+)}$	0,00628	0,01587	0,02245	0,03027

uncertainty is 10%, but for $Z = 130$ it reaches 30–60%. The corrections $\Delta E^{(3+)}$ are small in comparison with $\Delta E^{(1)}$, but they are much greater than the contribution $\Delta E^{(2)}_{\text{rad}}$ of the radiative corrections which are of order α^2. Thus, for the $1s$ state and $Z = 100$, the ratio $\Delta E^{(1)}:\Delta E^{(3+)}:\Delta E^{(2)}_{\text{rad}}$ is 400:20:1. In previous publications, the uncertainty in the estimated $\Delta E^{(3+)}$ was one of the main sources of uncertainty in the theoretical values of the energy levels.[3] This uncertainty is removed by the data given in Table II, so that the principal uncertainty in the calculations is now related only to the finite size of the nucleus.

In general, the finite size of the nucleus must be taken into account in the calculation of vacuum polarization as well. This is important for estimates of $\Delta E^{(1)}$, but can be omitted from $\Delta E^{(3+)}$ because $\Delta E^{(3+)}$ is itself small (the contribution due to the finite size of the nucleus to $V^{(3+)}$ was estimated in Refs. 10 and 12). Of course, as Z approaches 137, the results obtained for the $j = \frac{1}{2}$, which diverge for $\alpha Z = 1$ [see (26)], will not be valid for real ions.

In conclusion, we reproduce the corrections $\Delta E^{(1)}$, $\Delta E^{(3)}$, and $\Delta E^{(3+)}$ corresponding to the Uehling potential $V^{(1)}$, the Blomqvist potential $V^{(3)}$ (Ref. 6), and our calculated potential $V^{(3+)}$ for the ground state of ions with $Z = 55$, 82, 92, and 100 (Table III). We note that the values of $\Delta E^{(3)}$ given in Table III of Ref. 3 were used as estimates for $\Delta E^{(3+)}$.

APPENDIX

The derivatives

$$M'_{\pm 1/2,k}(x) = \frac{d}{d\eta} M_{\eta\pm 1/2,k}(x)\,|_{\eta=0},$$

$$W'_{\pm 1/2,k}(x) = \frac{d}{d\eta} W_{\eta\pm 1/2,k}(x)\,|_{\eta=0}$$

were calculated using the following expansions:

$$M'_{1/2-n,k}(x) = e^{-x/2}\sum_{m=1}^{\infty} \frac{(n+k)_m x^{m+k+1/2}}{(2k+1)_m m!}\,[\psi(n+k)-\psi(n+k+m)], \tag{A1}$$

$$W_{1/2-n,k}(x) = e^{-x/2}\Bigg\{\frac{(-1)^{k+n}}{(k-n+1)_k}\sum_{m=0}^{\infty} \frac{(k+n)_m x^{m+k+1/2}}{(2k+1)_m m!} \times [\ln x - \psi(m+1) + \psi(k+n+m) - \psi(2k+2m+1)]$$

$$+\sum_{m=0}^{k-n} \frac{(k+n)_m (k-n-m+1)_m}{m! x^{n+m-1/2}}[\psi(k+n) + \psi(k-n+1) - \psi(m+1)]$$

$$+\sum_{m=0}^{k+n-2} \frac{(-1)^m m! x^{m-n+1/2}}{(k-n+1)_{m+1}(k+n-m-1)_{m+1}}\Bigg\}, \tag{A2}$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$.

The formulas given by (A1) and (A2) were obtained by term-by-term differentiation of the expressions for M and W with an integer parameter.[14] For large x, we used the asymptotic expansion

$$W'_{1/2-n,k}(x) = e^{-x/2}\Bigg\{\sum_{m=0}^{k-n} \frac{(k+n)_m (k-n-m+1)_m}{m! x^{n+m-1/2}} \times \Bigg[\sum_{l=0}^{m-1}\left(\frac{1}{k-n-l} - \frac{1}{k+n+l}\right) + \ln x\Bigg] + \sum_{m=k-n+1}^{\infty} \frac{(-1)^{m+k-n}(k+n)_m (k-n)!}{(m+n-k)_{k-n+1} x^{m+n-1/2}}\Bigg\}, \tag{A3}$$

and also the expressions for M in terms of W' and W:

$$M'_{1/2-n,k}(x) = \frac{(-1)^{k+n}(2k)!}{(k-n)!}[W'_{1/2-n,k}(x) - \psi(k-n+1) W_{1/2-n,k}(x)] - \frac{(-1)^{k+n+1} e^x (2k)!}{(k+n-1)!}[W'_{n-1/2,k}(-x) - \psi(k+n) W_{n-1/2,k}(-x)].$$

Whenever the upper limit of summation is smaller than the lower, the corresponding sum is omitted.

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